# Low-energy moments of non-diagonal quark current correlators at four loops

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# Abstract

We compute the leading four physical terms in the low-energy expansions of heavy-light quark current correlators at four-loop order. As a by-product we reproduce the corresponding top-induced non-singlet correction to the electroweak  $\rho$  parameter.

Keywords: Perturbative calculations, Quantum Chromodynamics, Heavy Quarks

PACS: 12.38.Bx, 14.65.-q

#### 1. Introduction

Two-point correlation functions of heavy-light quark currents have found use in a number of phenomenological applications. One example is the prediction of corrections to the electroweak  $\rho$  parameter [1, 2, 3], where the flavour non-diagonal correlator of vector currents is required for vanishing external momentum. Another important class of applications is the sum-rule determination of meson decay constants (see e.g. [4, 5]). Here, the absorptive part of the respective correlators above the production threshold is needed.

Progress in lattice simulation may allow precise determinations of even more QCD parameters. For instance, the values of the strong coupling constant, the charm quark mass and the bottom quark mass have been determined with high accuracy from moments of heavy-heavy correlators in [6, 7]. In these analyses, moments of flavour diagonal currents have been determined on the lattice choosing a frame where the spatial momentum of the correlators vanishes.

The values of the quark masses and the coupling constant are then extracted by equating these moments to their counterparts calculated in perturbation theory at the four-loop order [8, 9, 10, 11, 12, 13, 14].

The methodology is thus similar to traditional quarkonium sum rules [15, 16, 17], but using lattice moments in place of moments of the experimentally measured hadronic R ratio. While for the sum rules only the correlator of vector currents can be used, there is no such restriction for the lattice simulation. In fact, in [6] different Lorentz structures were considered, with the most precise results stemming from pseudoscalar currents. Furthermore, also correlators of heavy-light currents could be used to extract the values of the charm and bottom quark masses and possibly the strong coupling constant [18]. To be competitive with the analyses for the heavy-heavy case the corrections to the perturbative moments of the heavy-light current correlators have to be known up to four loops. These corrections are presented in this work.

Given their usefulness, perturbative corrections to heavy-light correlators have been studied quite intensively and analytic results up to two loops have been known for many years [19, 20]. While the three-loop correction is not known analytically, many terms in expansions in both the low-energy and the high-energy limit have been calculated in [21, 22, 23]. Combining these with the behaviour near threshold, accurate approximations for arbitrary kinematics have been constructed [21, 22]. In the low-energy region also corrections due to a non-vanishing light quark mass are known [24, 25].

The four-loop corrections remain mostly unknown. In the high-energy region the leading term is equal to the non-singlet part of the corresponding diagonal correlator, which has been computed for both scalar and vector currents [26, 27, 28]. In the low-energy region, conversely, there is no such simple correspondence between diagonal and non-diagonal correlators. The vector correlator in the limit of vanishing external momentum constitutes a central ingredient in the determination of non-singlet four-loop corrections to the  $\rho$  parameter, which have been calculated in [2, 3].

In this work we present the four-loop corrections to the low-energy expansions of both scalar and vector heavy-light quark current correlators up to the eighth power of the external momentum. After introducing our conventions in section 2, we briefly describe the calculational setup and present our results in section 3. Section 4 describes the re-calculation of the top-induced contributions to the electroweak  $\rho$  parameter, which constitutes an important consistency check. We conclude in section 5.

# 2. Conventions

The correlators of heavy-light vector and scalar currents are defined as

$$\Pi_{\mu\nu}(q) = i \int dx \, e^{iqx} \langle 0|j_{\mu}(x)j_{\nu}(0)|0\rangle \,, \tag{1}$$

$$\Pi(q) = i \int dx \, e^{iqx} \langle 0|j(x)j(0)|0\rangle \tag{2}$$

with the vector current  $j_{\mu}(x) = \bar{\psi}(x)\gamma_{\mu}\chi(0)$  and the scalar current  $j(x) = \bar{\psi}(x)\chi(0)$ . We consider a heavy quark  $\psi$  with the pole mass m and a massless light quark  $\chi$ . It should be noted that in the limit of a vanishing light-quark mass the correlators of two axial-vector or pseudo-scalar currents coincide with the vector and scalar correlators, respectively.

It is convenient to introduce polarisation functions

$$\Pi_{\mu\nu}(q) = (-q^2 g_{\mu\nu} + q_{\mu} q_{\nu}) \Pi^{\nu}(q^2) + q_{\mu} q_{\nu} \Pi^{\nu}_L(q^2), \qquad (3)$$

$$\Pi(q) = q^2 \Pi^s(q^2) \,. \tag{4}$$

In the following we will not consider the longitudinal polarisation  $\Pi_L^v(q^2)$ . The perturbative expansions of  $\Pi^{\delta}(q^2)$  with  $\delta = v, s$  up to four loops read

$$\Pi^{\delta}(q^2) = \Pi^{\delta,(0)}(q^2) + \frac{\alpha_s}{\pi} C_F \Pi^{\delta,(1)}(q^2) + \left(\frac{\alpha_s}{\pi}\right)^2 \Pi^{\delta,(2)}(q^2) + \left(\frac{\alpha_s}{\pi}\right)^3 \Pi^{\delta,(3)}(q^2) + \dots$$
(5)

Being interested in the limit  $q^2 \to 0$ , we can expand the coefficients in the above series as

$$\Pi^{\delta,(i)}(q^2) = \frac{3}{16\pi^2} \sum_{n=-1}^{\infty} C_n^{\delta,(i)} z^n = \frac{3}{16\pi^2} \sum_{n=-1}^{\infty} \bar{C}_n^{\delta,(i)} \bar{z}^n,$$
 (6)

where we have used the abbreviations  $z=q^2/m^2, \bar{z}=q^2/\bar{m}^2$  with  $\bar{m}$  denoting the mass of the heavy quark in the  $\overline{\rm MS}$  scheme. Note that the coefficients with n=-1,0 still contain poles in the limit  $\epsilon=(4-d)/2\to 0$ . In physical observables these have to be cancelled by the wave-function and mass renormalisations of the particles (e.g. W bosons) coupling to the respective current. In the following we will describe the calculation of the coefficients  $C_n^{\delta,(3)}, \bar{C}_n^{\delta,(3)}$  for  $n\leq 4$ .

# 3. Calculation and results

First, the four-loop diagrams contributing to the polarisation functions are generated with QGRAF [29]. In the following steps we perform several algebraic manipulations with the help of TFORM [30, 31]. As a first simplification, we apply partial fractioning to denominators that differ only by their mass and the external momentum q, i.e. we use

$$\frac{1}{p^2} \frac{1}{(p \pm q)^2 - m^2} = \frac{1}{q^2 \pm 2pq - m^2} \left( \frac{1}{p^2} - \frac{1}{(p \pm q)^2 - m^2} \right). \tag{7}$$

Since we will perform an expansion in q the prefactor on the right-hand side has no influence on the tadpole topology of the considered diagram. Performing partial fractioning before the identification of the diagram topologies greatly reduces both the number and the complexity of the topologies that have to be considered. Using the algorithm described in Appendix A we map the resulting diagrams onto 28 topologies.

Next, colour factors are calculated using the FORM [30] package color [32]. We choose a routing for the external momentum q which minimizes the number of propagators depending on q. After this we evaluate the traces over gamma matrices and perform a Taylor expansion in q. The scalar integrals we obtain after tensor reduction and the elimination of reducible scalar products are reduced to master integrals using a private implementation<sup>1</sup> [35] of Laporta's algorithm [36]. All required master integrals are known analytically or numerically [37, 38, 39].

For the presentation of our results we impose the overall renormalisation condition  $\Pi^{v}(0) = \Pi^{s}(0) = 0$ . The corresponding divergent subtraction terms are listed in Appendix B. For the remaining coefficients according to equation (6) we obtain<sup>2</sup>

$$C_{1}^{v,(3)} = + 14.5508 C_{A}^{2} C_{F} + 8.4892 C_{A} C_{F}^{2} + 0.351 C_{F}^{3}$$

$$- 0.2294 C_{A} C_{F} T_{F} n_{h} - 0.6242 C_{F}^{2} T_{F} n_{h}$$

$$- 12.56835 C_{A} C_{F} T_{F} n_{l} - 3.07525 C_{F}^{2} T_{F} n_{l}$$

$$+ 0.107 C_{F} T_{F}^{2} n_{h}^{2} + 0.14 C_{F} T_{F}^{2} n_{h} n_{l} + 1.91917 C_{F} T_{F}^{2} n_{l}^{2}, \qquad (8)$$

$$C_{2}^{v,(3)} = + 7.39116 C_{A}^{2} C_{F} + 5.65943 C_{A} C_{F}^{2} + 0.80504 C_{F}^{3}$$

$$+ 0.0683 C_{A} C_{F} T_{F} n_{h} - 0.3114 C_{F}^{2} T_{F} n_{h}$$

$$- 6.0806 C_{A} C_{F} T_{F} n_{l} - 2.2303 C_{F}^{2} T_{F} n_{l}$$

$$+ 0.008 C_{F} T_{F}^{2} n_{h}^{2} - 0.0052 C_{F} T_{F}^{2} n_{h} n_{l} + 0.9442 C_{F} T_{F}^{2} n_{l}^{2}, \qquad (9)$$

$$C_{3}^{v,(3)} = + 4.42563 C_{A}^{2} C_{F} + 3.86666 C_{A} C_{F}^{2} + 0.73105 C_{F}^{3}$$

$$+ 0.0448 C_{A} C_{F} T_{F} n_{h} - 0.1713 C_{F}^{2} T_{F} n_{h}$$

$$- 3.57037 C_{A} C_{F} T_{F} n_{l} - 1.5461 C_{F}^{2} T_{F} n_{l}$$

$$+ 0.0017 C_{F} T_{F}^{2} n_{h}^{2} - 0.005 C_{F} T_{F}^{2} n_{h} n_{l} + 0.56396 C_{F} T_{F}^{2} n_{l}^{2}, \qquad (10)$$

$$C_{4}^{v,(3)} = + 2.90512 C_{A}^{2} C_{F} + 2.7515 C_{A} C_{F}^{2} + 0.5965 C_{F}^{3}$$

$$+ 0.0278 C_{A} C_{F} T_{F} n_{h} - 0.104 C_{F}^{2} T_{F} n_{h}$$

$$- 2.31867 C_{A} C_{F} T_{F} n_{l} - 1.10502 C_{F}^{2} T_{F} n_{l}$$

$$+ 0.0006 C_{F} T_{F}^{2} n_{h}^{2} - 0.003 C_{F} T_{F}^{2} n_{h} n_{l} + 0.3708 C_{F} T_{F}^{2} n_{l}^{2}, \qquad (11)$$

$$C_{1}^{v,(3)} = + 1.6424 C_{A}^{2} C_{F} + 1.65318 C_{A} C_{F}^{2} + 1.41042 C_{F}^{3}$$

$$- 1.39916 C_{A} C_{F} T_{F} n_{h} + 0.556834 C_{F}^{2} T_{F} n_{h}$$

$$- 3.129699 C_{A} C_{F} T_{F} n_{l} + 0.556834 C_{F}^{2} T_{F} n_{h} + 0.441495 C_{F} T_{F}^{2} n_{l}^{2}, \qquad (12)$$

<sup>&</sup>lt;sup>1</sup> The implementation is written in C++ and uses GiNaC [33] and fermat [34].

<sup>&</sup>lt;sup>2</sup>The moments are presented in a form that yields five significant digits for QCD with  $n_l \leq 5$  light flavours. All results are attached in electronic form as ancillary files to this preprint.

$$C_{2}^{s,(3)} = +5.66925 C_{A}^{2} C_{F} + 5.36995 C_{A} C_{F}^{2} + 2.1099 C_{F}^{3}$$

$$-0.0476 C_{A} C_{F} T_{F} n_{h} + 0.1338 C_{F}^{2} T_{F} n_{h}$$

$$-5.00716 C_{A} C_{F} T_{F} n_{l} - 1.60465 C_{F}^{2} T_{F} n_{l}$$

$$+0.037 C_{F} T_{F}^{2} n_{h}^{2} + 0.0314 C_{F} T_{F}^{2} n_{h} n_{l} + 0.711301 C_{F} T_{F}^{2} n_{l}^{2}, \qquad (13)$$

$$C_{3}^{s,(3)} = +4.18695 C_{A}^{2} C_{F} + 4.9201 C_{A} C_{F}^{2} + 2.0783 C_{F}^{3}$$

$$+0.0196 C_{A} C_{F} T_{F} n_{h} - 0.0103 C_{F}^{2} T_{F} n_{h}$$

$$-3.5077 C_{A} C_{F} T_{F} n_{l} - 1.7089 C_{F}^{2} T_{F} n_{l}$$

$$+0.009 C_{F} T_{F}^{2} n_{h}^{2} + 0.0006 C_{F} T_{F}^{2} n_{h} n_{l} + 0.5215 C_{F} T_{F}^{2} n_{l}^{2}, \qquad (14)$$

$$C_{4}^{s,(3)} = +2.945114 C_{A}^{2} C_{F} + 3.81782 C_{A} C_{F}^{2} + 1.6905 C_{F}^{3}$$

$$+0.01994 C_{A} C_{F} T_{F} n_{h} - 0.0347 C_{F}^{2} T_{F} n_{h}$$

$$-2.41729 C_{A} C_{F} T_{F} n_{l} - 1.3927 C_{F}^{2} T_{F} n_{l}$$

$$+0.0034 C_{F} T_{F}^{2} n_{h}^{2} - 0.0016 C_{F} T_{F}^{2} n_{h} n_{l} + 0.36976 C_{F} T_{F}^{2} n_{l}^{2}, \qquad (15)$$

where we have set the renormalisation scale  $\mu$  to the on-shell mass m. We follow the usual convention for the colour factors with  $C_A = 3$ ,  $C_F = 4/3$ ,  $T_f = 1/2$  for QCD. The number of light (massless) quark flavours is denoted by  $n_l$ , whereas  $n_h$  stands for the number of heavy flavours.

If we choose to express the polarisation functions in terms of the  $\overline{\text{MS}}$  mass  $\bar{m}$  at the scale  $\mu = \bar{m}$  and  $\alpha_s(\bar{m})$ , we arrive at

$$\begin{split} \bar{C}_{1}^{v,(3)} &= -1.2994791\,C_{A}^{2}C_{F} + 1.20957\,C_{A}C_{F}^{2} + 0.537098\,C_{F}^{3} \\ &- 1.75125\,C_{A}C_{F}T_{F}n_{h} + 1.29201\,C_{F}^{2}T_{F}n_{h} \\ &+ 0.530618\,C_{A}C_{F}T_{F}n_{l} - 0.0193\,C_{F}^{2}T_{F}n_{l} \\ &- 0.0853\,C_{F}T_{F}^{2}n_{h}^{2} + 0.07322\,C_{F}T_{F}^{2}n_{h}n_{l} - 0.0389\,C_{F}T_{F}^{2}n_{l}^{2}\,, \end{split} \tag{16}$$

$$\bar{C}_{2}^{v,(3)} &= -1.0623284\,C_{A}^{2}C_{F} + 1.035507\,C_{A}C_{F}^{2} + 0.1608\,C_{F}^{3} \\ &- 0.74336\,C_{A}C_{F}T_{F}n_{h} + 0.72663\,C_{F}^{2}T_{F}n_{h} \\ &+ 0.905515\,C_{A}C_{F}T_{F}n_{l} - 0.46186\,C_{F}^{2}T_{F}n_{l} \\ &- 0.0944796\,C_{F}T_{F}^{2}n_{h}^{2} - 0.04078\,C_{F}T_{F}^{2}n_{h}n_{l} - 0.10011\,C_{F}T_{F}^{2}n_{l}^{2}\,, \end{split} \tag{17}$$

$$\bar{C}_{3}^{v,(3)} &= -0.8577978\,C_{A}^{2}C_{F} + 1.1607802\,C_{A}C_{F}^{2} - 0.1496539\,C_{F}^{3} \\ &- 0.4624948\,C_{A}C_{F}T_{F}n_{h} + 0.520167\,C_{F}^{2}T_{F}n_{h} \\ &+ 0.7959545\,C_{A}C_{F}T_{F}n_{l} - 0.631599\,C_{F}^{2}T_{F}n_{l} \\ &- 0.06236\,C_{F}T_{F}^{2}n_{h}^{2} - 0.027228\,C_{F}T_{F}^{2}n_{h}n_{l} - 0.08873276\,C_{F}T_{F}^{2}n_{l}^{2}\,, \end{split} \tag{18}$$

$$\bar{C}_{4}^{v,(3)} &= -0.717803\,C_{A}^{2}C_{F} + 1.286187\,C_{A}C_{F}^{2} - 0.40493\,C_{F}^{3} \\ &- 0.320038\,C_{A}C_{F}T_{F}n_{h} + 0.41065\,C_{F}^{2}T_{F}n_{h} \\ &+ 0.67538025\,C_{A}C_{F}T_{F}n_{l} - 0.72124\,C_{F}^{2}T_{F}n_{l} \\ &- 0.04337\,C_{F}T_{F}^{2}n_{h}^{2} - 0.018157\,C_{F}T_{F}^{2}n_{h}n_{l} - 0.076781\,C_{F}T_{F}^{2}n_{l}^{2}\,, \end{split} \tag{19}$$

$$\begin{split} \bar{C}_{1}^{s,(3)} &= + 1.642401 \, C_{A}^{2}C_{F} - 0.510074 \, C_{A}C_{F}^{2} + 1.41042 \, C_{F}^{3} \\ &- 1.39916 \, C_{A}C_{F}T_{F}n_{h} + 1.34177 \, C_{F}^{2}T_{F}n_{h} \\ &- 3.1297 \, C_{A}C_{F}T_{F}n_{l} + 1.343472 \, C_{F}^{2}T_{F}n_{l} \\ &+ 0.3759 \, C_{F}T_{F}^{2}n_{h}^{2} + 0.65308 \, C_{F}T_{F}^{2}n_{h}n_{l} + 0.4415 \, C_{F}T_{F}^{2}n_{l}^{2} \,, \end{split}$$
 (20) 
$$\bar{C}_{2}^{s,(3)} &= + 0.38582 \, C_{A}^{2}C_{F} + 0.31725 \, C_{A}C_{F}^{2} + 0.916757 \, C_{F}^{3} \\ &- 0.55487 \, C_{A}C_{F}T_{F}n_{h} + 0.80004 \, C_{F}^{2}T_{F}n_{h} \\ &- 0.640838 \, C_{A}C_{F}T_{F}n_{l} + 0.44938 \, C_{F}^{2}T_{F}n_{l} \\ &- 0.02698 \, C_{F}T_{F}^{2}n_{h}^{2} + 0.0092 \, C_{F}T_{F}^{2}n_{h}n_{l} + 0.05861 \, C_{F}T_{F}^{2}n_{l}^{2} \,, \end{split}$$
 (21) 
$$\bar{C}_{3}^{s,(3)} &= -0.039796 \, C_{A}^{2}C_{F} + 0.48671411 \, C_{A}C_{F}^{2} + 0.4018122 \, C_{F}^{3} \\ &- 0.38621 \, C_{A}C_{F}T_{F}n_{h} + 0.46308 \, C_{F}^{2}T_{F}n_{h} \\ &- 0.014653 \, C_{A}C_{F}T_{F}n_{l} + 0.042405 \, C_{F}^{2}T_{F}n_{l} \\ &- 0.0422 \, C_{F}T_{F}^{2}n_{h}^{2} - 0.01723 \, C_{F}T_{F}^{2}n_{h}n_{l} - 0.00067 \, C_{F}T_{F}^{2}n_{l}^{2} \,, \end{split}$$
 (22) 
$$\bar{C}_{4}^{s,(3)} &= -0.224943 \, C_{A}^{2}C_{F} + 0.565757 \, C_{A}C_{F}^{2} + 0.067439 \, C_{F}^{3} \\ &- 0.284427 \, C_{A}C_{F}T_{F}n_{h} + 0.3319473 \, C_{F}^{2}T_{F}n_{h} \\ &+ 0.2025025 \, C_{A}C_{F}T_{F}n_{l} - 0.162445 \, C_{F}^{2}T_{F}n_{l} \\ &- 0.035056 \, C_{F}T_{F}^{2}n_{h}^{2} - 0.014915 \, C_{F}T_{F}^{2}n_{h}n_{l} - 0.021858 \, C_{F}T_{F}^{2}n_{l}^{2} \,. \end{split}$$

# 4. The $\rho$ parameter

To verify the correctness of our calculation we have performed a number of cross checks. Obviously, our results are UV-finite. We have also performed an expansion up to linear order in the gauge parameter and verified that the gauge dependence cancels in the coefficients  $\bar{C}_1^{v,(3)}, \bar{C}_1^{s,(3)}$ . The strongest check, however, is the comparison to the known four-loop non-singlet corrections to the  $\rho$  parameter [2, 3].

The electroweak  $\rho$  parameter has been introduced in Ref. [40]. Considering only QCD corrections it can be written as

$$\rho = 1 + \delta \rho \tag{24}$$

with

$$\delta \rho = \frac{\Pi_{ZZ}(0)}{M_Z^2} - \frac{\Pi_{WW}(0)}{M_W^2} \,, \tag{25}$$

where  $\Pi_{ZZ}(0)$  and  $\Pi_{WW}(0)$  denote the self energies of Z and W boson, respectively.

In order to calculate the contribution from the Z-boson self energy to the  $\rho$  parameter we also need the leading moment of the flavour diagonal correlator. To this end we introduce  $\Pi^a_{\text{diag}}(q^2)$  similar to Eq. (1) but with the heavy-heavy axial current

$$\tilde{j}_a^{\mu} = \bar{\psi}\gamma_5\gamma^{\mu}\psi\,,$$
(26)

and the moments

$$\Pi_{\text{diag}}^{a,(3)}(q^2) = \frac{3}{16\pi^2} \sum_{n=-1}^{\infty} C_n^{a,(3)} \left(\frac{q^2}{4m^2}\right)^n.$$
 (27)

In what follows we will only consider the top-induced four-loop correction to  $\rho$ , corresponding to  $\rho_3$  in the expansion

$$\delta \rho = 3x_t \sum_{i=0}^{\infty} \left(\frac{\alpha_s}{\pi}\right)^i \rho_i, \qquad x_t = \frac{\sqrt{2}G_F m_t^2}{16\pi^2}. \tag{28}$$

The corresponding corrections to the Z and W self energies then read

$$\frac{\Pi_{ZZ}^{(3)}(0)}{M_Z^2} = 3x_t \left[ \left( 1 - \frac{1}{d} \right) C_{-1,\text{diag}}^{a,(3)} - \frac{1}{d} C_{L,-1,\text{diag}}^{a,(3)} \right] + \text{singlet terms},$$
(29)

and

$$\frac{\Pi_{WW}^{(3)}(0)}{M_W^2} = 3x_t \left[ \left( 1 - \frac{1}{d} \right) C_{-1}^{v,(3)} - \frac{1}{d} C_{L,-1}^{v,(3)} \right], \tag{30}$$

where the higher-order corrections  $\Pi^{(3)}_{ZZ}, \Pi^{(3)}_{WW}$  are defined in analogy to equation (5).  $C^{v,(3)}_{L,-1}$  and  $C^{a,(3)}_{L,-1,\text{diag}}$  denote the moments with n=-1 of the respective longitudinal polarisation functions; from an explicit calculation we obtain

$$C_{L,-1}^{v,(3)} = -C_{-1}^{v,(3)}, \qquad C_{L,-1,\text{diag}}^{a,(3)} = -C_{-1,\text{diag}}^{a,(3)}.$$
 (31)

Note that in the non-diagonal case the vector and axial-vector correlators conincide and that the (-1)-th moment of the diagonal vector correlator vanishes. The contributions from W- and Z-boson self energies are divergent on their own and only their sum is finite. The singlet terms calculated in Ref. [1] are finite on their own and we do not repeat them here. Using the results given in Appendix B we obtain in the  $\overline{\rm MS}$  scheme

$$\bar{\rho}_{3,\text{non-singlet}} = \bar{C}_{-1,\text{diag}}^{a,(3)} - \bar{C}_{-1}^{v,(3)} = 1.60667,$$
(32)

and after converting to the on-shell scheme

$$\rho_{3,\text{non-singlet}} = -101.083,$$
(33)

in full agreement with the results in the literature [2, 3].

### 5. Conclusion

We have calculated the four-loop QCD corrections to the low-energy moments of flavour non-diagonal current correlators up to n = 4. Our results are

valid for (axial-)vector and (pseudo-)scalar currents in the limit of a vanishing light-quark mass. As a by-product we have confirmed the results for the non-singlet correction to the electroweak  $\rho$  parameter first obtained in [2, 3]. In combination with lattice simulations, our results can be used for the precision determination of heavy-quark masses. Furthermore, they can serve as an ingredient in the approximate reconstruction of the four-loop corrections for arbitrary external momenta. For the latter application, however, more input from other kinematic regions is still required.

## Acknowledgments

This work was supported by European Commission through contract PITN-GA-2012-316704 (HIGGSTOOLS). We would like to thank Matthias Steinhauser for the reading of the manusript.

# Appendix A. Symmetrisation

The closely related problems of symmetrisation and mapping diagrams to topologies are ubiquitous in multiloop calculations. Commonly used algorithms employ either the diagrams' parametric representations [41] or representations as graphs. To avoid cumbersome transformations, we choose to work with the original algebraic form obtained directly from the Feynman rules.

A general L-loop scalar diagram I with P propagators has the form

$$I = \int [dl_1] \dots [dl_L] \frac{1}{D_1^{a_1} \dots D_D^{a_P}}$$
 (A.1)

with (not necessarily positive) integers  $a_1, \ldots a_P$ . The  $[dl_i]$  are suitable d-dimensional integral measures, e.g. as in equation (B.1), and the propagators  $D_i$  are functions of the loop momenta  $l_1, \ldots, l_L$ , any number of external momenta, and a mass  $m_i$ . Obviously, I is invariant under a change of variables

$$\mathcal{M}: l_i \mapsto l_i' = M_{ij}l_j + q_i \tag{A.2}$$

with  $|\det(M)| = 1$  and constant vectors  $q_i$ .

Consider now a diagram  $\tilde{I}$  with propagators  $\tilde{D}_1, \ldots, \tilde{D}_P$  and the diagram I as defined by eq. (A.1). Let us denote the propagators we obtain by changing the loop momenta in I according to eq. (A.2) as  $D'_1, \ldots, D'_P$ . We say that I and  $\tilde{I}$  belong to the same topology iff there is a transformation  $\mathcal{M}$  such that  $\{D'_1, \ldots, D'_P\} = \{\tilde{D}_1, \ldots, \tilde{D}_P\}$ . Likewise, I belongs to a subtopology of  $\tilde{I}$  iff for some  $\mathcal{M}$  we have  $\{D'_1, \ldots, D'_P\} \subseteq \{\tilde{D}_1, \ldots, \tilde{D}_P\}$ . The problem of mapping a diagram to a topology thus reduces to finding out whether a suitable transformation  $\mathcal{M}$  exists.

The basic idea behind our algorithm is to first look for L propagators  $D_i$  that depend on all loop momenta  $l_1, \ldots, l_L$ . Then we select L appropriate mutually different target propagators  $\tilde{D}_{j_i}$  and define  $\mathcal{M}$  such that  $D'_i = \tilde{D}_{j_i}$ . If the sets of

the remaining propagators are also equal after applying  $\mathcal{M}$ , the two topologies are the same.

To be more concrete, let us now consider a diagram I defined as in equation (A.1) with propagators of the form  $D_i = p_i^2 \pm m_i^2$ , where the  $p_i$  are linear combinations of loop momenta and external momenta. The generalisation to other forms of the propagators should be straightforward. In practice, we can choose the first L propagators to be of the form  $D_i = l_i^2 \pm m_i^2$ . The algorithm then works as follows.

- 1. Select a new target topology and choose a representative with propagators  $\{\tilde{D}_1, \dots, \tilde{D}_P\}$  of the form  $\tilde{D}_i = \tilde{p}_i^2 \pm \tilde{m}_i^2$  from it.
- 2. Choose a tuple  $(\tilde{D}_{i_1}, \ldots, \tilde{D}_{i_L})$  (that was not chosen before) of L distinct propagators with compatible masses, i.e.  $\tilde{m}_{i_1} = m_1, \ldots, \tilde{m}_{i_L} = m_L$ . If this is not possible go back to step 1.
- 3. Consider the next among the  $2^L$  transformations that map the propagators  $(D_1, \ldots, D_L)$  onto  $(\tilde{D}_{i_1}, \ldots, \tilde{D}_{i_L})$ , i.e.  $l_j \mapsto \pm p_{i_j} j = 1, \ldots, L$ . If no transformation is left go back to step 2.
- 4. Apply the current transformation to the propagators  $D_1, \ldots, D_P$ . I then belongs to the current target topology if  $\{D'_1, \ldots, D'_P\} = \{\tilde{D}_1, \ldots, \tilde{D}_P\}$ . Else go back to step 3.

As far as identifying the topology of an integral is concerned the algorithm terminates as soon as step 4 is completed successfully. For symmetrisation we would skip step 1 and always go back from step 4 to step 3 in order to find all automorphisms.

# Appendix B. Subtraction terms

Since the leading coefficients with n = -1, 0 in equation (6) still depend on the dimensional regulator  $\epsilon = (4 - d)/2$ , we first have to specify our renormalisation prescriptions in d dimensions in order to give meaningful expressions.

Our d-dimensional integration measure is given by

$$[dl_i] = \frac{d^d l_i}{i\pi^{d/2}} e^{\epsilon \gamma_E} \,, \tag{B.1}$$

where  $\gamma_E \approx 0.5772157$  is the Euler-Mascheroni constant. The counterterms in the  $\overline{\rm MS}$  scheme are now defined such that they exactly cancel the poles in  $\epsilon$ . For the sake of simplicity, we refrain from defining on-shell renormalisation and present the divergent coefficients in terms of the  $\overline{\rm MS}$  quark mass. Writing

$$\bar{C}_n^{\delta,(3)} = \sum_{i=0}^{3-n} \frac{\bar{c}_{n,i}^{\delta,(3)}}{\epsilon^i}$$
 (B.2)

we obtain for  $\mu = \bar{m}$ 

$$\begin{split} \bar{c}_{-1,0}^{v,(3)} &= + 1.740 \, C_A^2 C_F - 9.555 \, C_A C_F^2 + 15.433 \, C_F^3 \\ &- 7.803 \, C_A C_F T_F n_h + 7.355 \, C_F^2 T_F n_h \\ &- 0.228 \, C_A C_F T_F n_l - 1.897 \, C_F^2 T_F n_l \\ &- 0.935 \, C_F T_F^2 n_h^2 + 0.735 \, C_F T_F^2 n_h n_l + 1.024 \, C_F T_F^2 n_l^2 \,, \\ \bar{c}_{-1,1}^{v,(3)} &= - 1.196 \, C_A^2 C_F + 0.592 \, C_A C_F^2 - 1.377 \, C_F^3 \\ &+ 1.130 \, C_A C_F T_F n_f + 0.015 \, C_F^2 T_F n_f + 0.009 \, C_F T_F^2 n_f^2 \,, \\ \bar{c}_{-1,2}^{v,(3)} &= + 2.195 \, C_A^2 C_F + 0.649 \, C_A C_F^2 + 1.278 \, C_F^3 \\ &- 1.623 \, C_A C_F T_F n_f - 0.244 \, C_F^2 T_F n_f - 0.025 \, C_F T_F^2 n_f^2 \,, \\ \bar{c}_{-1,3}^{v,(3)} &= - 1.058 \, C_A^2 C_F - 1.750 \, C_A C_F^2 - 0.352 \, C_F^3 \\ &+ 0.635 \, C_A C_F T_F n_f + 0.531 \, C_F^2 T_F n_f - 0.069 \, C_F T_F^2 n_f^2 \,, \\ \bar{c}_{-1,3}^{v,(3)} &= - 1.058 \, C_A^2 C_F - 1.750 \, C_A C_F^2 + 0.281 \, C_F^3 \\ &- 0.153 \, C_A C_F T_F n_f - 0.188 \, C_F^2 T_F n_f + 0.028 \, C_F T_F^2 n_f^2 \,, \\ \bar{c}_{-1,3}^{v,(3)} &= - 0.832 \, C_A^2 C_F - 3.606 \, C_A C_F^2 + 2.628 \, C_F^3 \\ &- 0.432 \, C_A C_F T_F n_f + 0.188 \, C_F^2 T_F n_f + 0.028 \, C_F T_F^2 n_f^2 \,, \\ \bar{c}_{0,0}^{v,(3)} &= - 0.832 \, C_A^2 C_F - 3.606 \, C_A C_F^2 - 2.180 \, C_F^3 \\ &- 1.432 \, C_A C_F T_F n_h + 2.335 \, C_F^2 T_F n_h \\ &+ 2.239 \, C_A C_F T_F n_h + 0.666 \, C_F^2 T_F n_h \\ &- 0.425 \, C_F T_F^2 n_h^2 - 0.479 \, C_F T_F^2 n_h n_l - 0.330 \, C_F T_F^2 n_f^2 \,, \\ \bar{c}_{0,1}^{v,(3)} &= + 0.277 \, C_A^2 C_F + 0.065 \, C_A C_F^2 - 0.180 \, C_F^3 \\ &- 0.417 \, C_A C_F T_F n_f + 0.172 \, C_F^2 T_F n_f - 0.020 \, C_F T_F^2 n_f^2 \,, \\ \bar{c}_{0,2}^{v,(3)} &= - 0.230 \, C_A^2 C_F + 0.019 \, C_A C_F^2 \\ &+ 0.150 \, C_A C_F T_F n_f + 0.172 \, C_F^2 T_F n_f + 0.009 \, C_F T_F^2 n_f^2 \,, \\ \bar{c}_{0,1}^{v,(3)} &= + 0.777 \, C_A^2 C_F - 114.585 \, C_A C_F^2 + 20.766 \, C_F^3 \\ &+ 14.819 \, C_A C_F T_F n_h + 101.776 \, C_F^2 T_F n_h \\ &+ 62.816 \, C_A C_F T_F n_h + 101.776 \, C_F^2 T_F n_h \\ &+ 62.816 \, C_A C_F T_F n_h + 101.776 \, C_F^2 T_F n_h \\ &- 17.829 \, C_F T_F^2 n_h^2 - 24.041 \, C_F T_F^2 n_h n_l - 3.175 \, C_F T_F^2 n_l^2 \,, \\ &+ 16.536 \, C_A C_F T_F n_h - 0.5$$

$$\begin{split} \bar{c}_{-1,2}^{s,(3)} &= + 7.939\,C_A^2C_F + 1.310\,C_AC_F^2 + 3.731\,C_F^3 \\ &- 7.673\,C_AC_FT_Fn_h - 3.327\,C_F^2T_Fn_h \\ &- 5.840\,C_AC_FT_Fn_l - 0.327\,C_F^2T_Fn_l \\ &+ 0.481\,C_FT_F^2n_h^2 + 0.296\,C_FT_F^2n_hn_l - 0.185\,C_FT_F^2n_l^2 \,, \qquad (B.14) \\ \bar{c}_{-1,3}^{s,(3)} &= - 3.813\,C_A^2C_F - 11.708\,C_AC_F^2 - 2.438\,C_F^3 \\ &+ 2.236\,C_AC_FT_Fn_f + 3.042\,C_F^2T_Fn_f - 0.222\,C_FT_F^2n_f^2 \,, \qquad (B.15) \\ \bar{c}_{-1,4}^{s,(3)} &= + 0.840\,C_A^2C_F + 4.125\,C_AC_F^2 + 4.500\,C_F^3 \\ &- 0.611\,C_AC_FT_Fn_f - 1.500\,C_F^2T_Fn_f + 0.111\,C_FT_F^2n_f^2 \,, \qquad (B.16) \\ \bar{c}_{0,0}^{s,(3)} &= - 1.740\,C_A^2C_F + 9.555\,C_AC_F^2 - 15.433\,C_F^3 \\ &+ 7.803\,C_AC_FT_Fn_h - 7.355\,C_F^2T_Fn_h \\ &+ 0.228\,C_AC_FT_Fn_l + 1.897\,C_F^2T_Fn_l \\ &+ 0.935\,C_FT_F^2n_h^2 - 0.735\,C_FT_F^2n_hn_l - 1.024\,C_FT_F^2n_l^2 \,, \qquad (B.17) \\ \bar{c}_{0,1}^{s,(3)} &= + 1.196\,C_A^2C_F - 0.592\,C_AC_F^2 + 1.377\,C_F^3 \\ &- 1.130\,C_AC_FT_Fn_f - 0.015\,C_F^2T_Fn_f - 0.009\,C_FT_F^2n_f^2 \,, \qquad (B.18) \\ \bar{c}_{0,2}^{s,(3)} &= - 2.195\,C_A^2C_F - 0.649\,C_AC_F^2 - 1.278\,C_F^3 \\ &+ 1.623\,C_AC_FT_Fn_f + 0.244\,C_F^2T_Fn_f + 0.025\,C_FT_F^2n_f^2 \,, \qquad (B.19) \\ \bar{c}_{0,3}^{s,(3)} &= + 1.058\,C_A^2C_F + 1.750\,C_AC_F^2 + 0.352\,C_F^3 \\ &- 0.635\,C_AC_FT_Fn_f - 0.531\,C_F^2T_Fn_f + 0.069\,C_FT_F^2n_f^2 \,, \qquad (B.20) \\ \end{split}$$

with  $n_f = n_h + n_l$ .

In addition to the listed coefficient  $\bar{C}_{-1}^{v,(3)}$  we require the corresponding coefficient  $\bar{C}_{-1,\mathrm{diag}}^{a,(3)}$  in the low-energy expansion of the flavour diagonal axial-vector correlator in order to compute the correction to the  $\rho$  parameter. Since the pole parts of these two coefficients have to cancel, we can decompose the latter coefficient as

$$\bar{C}_{-1,\text{diag}}^{a,(3)} = \bar{C}_{-1,\text{diag}}^{a,(3)} \Big|_{\text{fin}} - \sum_{i=1}^{4} \frac{\bar{c}_{-1,i}^{v,(3)}}{\epsilon^{i}} \tag{B.21}$$

with the coefficients  $\bar{c}_{-1,i}^{v,(3)}$  as in equations B.4–B.7. The remaining finite part is given by

$$\begin{split} \bar{C}_{-1,\text{diag}}^{a,(3)} \bigg|_{\text{fin}} &= +2.484 \, C_A^2 C_F - 8.319 \, C_A C_F^2 + 16.954 \, C_F^3 \\ &- 5.300 \, C_A C_F T_F n_h + 2.759 \, C_F^2 T_F n_h \\ &- 1.598 \, C_A C_F T_F n_l - 4.210 \, C_F^2 T_F n_l \\ &- 0.247 \, C_F T_F^2 n_h^2 + 1.585 \, C_F T_F^2 n_h n_l + 1.492 \, C_F T_F^2 n_l^2 \,, \end{split} \tag{B.22}$$

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